

Si *L* X-Ray Emission Spectra of Cubic Silicon Molecules and Their Electronic Structures Analyzed by DV- $X\alpha$ Molecular Orbital Calculations

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Cubic silicon molecules are interesting materials from the viewpoint of advanced quantum electronic devices, because they are considered to be the minimum quantum silicon clusters. We therefore measured x-ray emission and absorption spectra of the octa-*tert*-butylpentacyclo [4.2.0.0^{2,5}.0^{3,8}.0^{4,7}] octasilane (denoted by “octasilacubane”) [1] and 1,2,3,4,5,6,7,8-octa-*tert*-butyltetracyclo [4.2.0.0^{2,5}.0^{3,8}] octasilane (“octasilasecucubane”) [2] in the Si *K* region to analyze their electronic structure [3]. Figure 1 shows the molecular structure of octasilacubane and octasilasecucubane. In order to further analyze the electronic structure of the octasilacubane and octasilasecucubane, we measured soft x-ray emission spectra of them in the Si *L* region using a grating x-ray spectrometer installed in BL-8.0.1, and analyzed the x-ray emission spectral features by discrete variational (DV) - $X\alpha$ molecular orbital calculations. Figure 2 shows the Si *L* x-ray emission spectra and calculated density of state (DOS) spectra. The Si *L* x-ray emission spectra of octasilacubane and octasilasecucubane can be approximately reproduced by the sum of the Si3s- and Si3d-DOSs. It is also demonstrated that the valence orbital structure of cubic silicon molecules is strongly dependent on the symmetry of the silicon backbones.

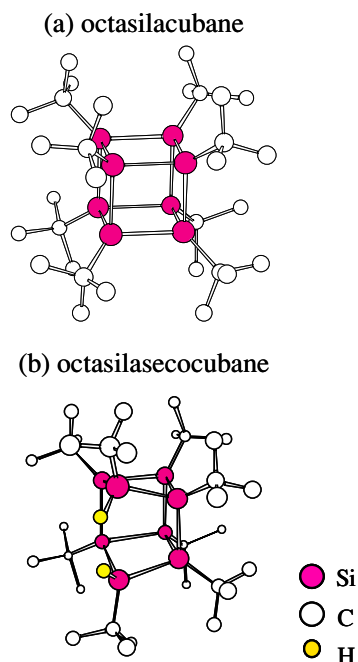


Figure 1. Molecular structures of (a) octasilacubane and (b) octasilasecucubane. Hydrogen atoms of *tert*-butyl substituents are not shown. Only the hydrogen atoms bonding directly to silicon backbone of octasilasecucubane are shown.

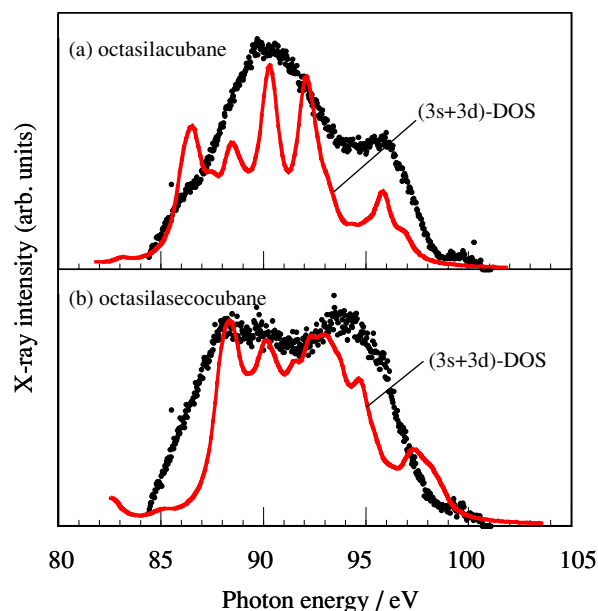


Figure 2. Si *L* x-ray emission spectra (dotted lines) of (a) octasilacubane and (b) octasilasecucubane, with superimposed calculated Si3s- and Si3d-DOS spectra (solid lines).

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